Methane, bis-(o-methoxyphenyl)-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.32e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 4.86e-01

Nearest Neighbors from the Training Set

Image not found
alpha-Santonin
Measured: 8.12e-04
Predicted: 5.45e-04

Image not found
Sparteine
Measured: 1.30e-02
Predicted: 8.29e-03

Image not found
Oxabentrinil
Measured: 8.61e-05
Predicted: 1.53e-03

Image not found
.alpha.-[(Cyanomethoxy)imino]benzeneacetonitrile
Measured: 5.13e-04
Predicted: 5.60e-02

Image not found
N-(1-Naphthyl)ethylenediamine
Measured: 1.07e-02
Predicted: 9.11e-02